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Artificial neural network model of a short stack solid oxide fuel cell based on experimental data

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HIGHLIGHTS

- Artificial neural network model for a SOFC trained by experimental data.
- Finding the optimized structure of the multi-layer back-propagation neural network.
- Experimental set up for current, voltage and temperature measurements of the SOFC stack.
- Prediction of the temperature profile and voltage of the SOFC.

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ABSTRACT

Solid oxide fuel cells (SOFCs) are complex systems in which electrical conduction, heat transfer, gas phase mass transport, chemical reactions and ionic conduction take place simultaneously and are tightly coupled. Mathematical models based on conservation laws have been shown to be slow and because of some parameter estimation for physical, chemical and electrochemical properties they have less accuracy. ANN models are powerful tools that bring simplicity and real-time response to SOFC modeling. Depending on the quality of the training data, ANN models can also show greater accuracy than CFD models. In this study ANN modeling of a short stack SOFC is considered. Training data are extracted and filtered from measurements on a dedicated test set-up. Given the fuel flow and composition, air flow, oven temperature and current, the model can predict the voltage and temperature profile of the cell. An optimized structure for the network is selected as: 5–11–6 for a 5 input, 6 output network with 11 hidden neurons. Prediction results of the ANN model deviate 0.2% concerning average relative error compared to the measurements.

1. Introduction

Ancient Persians invented the first battery 2000 years ago [1]. The application of their electrochemical source of energy is not clear for us, but today the electrochemical power sources and especially SOFCs are considered as the promising technologies for future energy demand. With electrical efficiencies that can reach over 50% [2–4], even in small power ranges, SOFC is the good competitor for other energy conversion technologies. Due to its high working temperature, a variety of fuels including fossil and renewable fuels, such as biogas, can be used with high efficiency for electricity and heat production [5–9]. There is an interest in combining pressurized SOFCs with gas turbines in hybrid cycles to achieve even higher efficiencies and lower emissions [7,10–15].

"A neural network is a parallel distributed processor made up of simple processing units that has a natural propensity for storing experimental knowledge and making it available for use" [16]. The artificial neural network (ANN) is a strong technique for modeling the complex non-linear systems without having the detailed mathematical formulation of the system. Similar to the human brain structure, the ANN has neurons, synaptic weights and activation functions among others. The network usually goes through a learning (training) process and the knowledge is stored in the synaptic weights of the network. In this process, input data are multiplied by synaptic weights then they are summed and processed in the neurons in order to generate an output.

The topic of ANNs has become very broad and, because of their flexibility, many structures have been suggested and used for a broad range of applications. However, the multilayer perceptron combined with error back-propagation has shown great performance in dealing with regression problems [17–21].

The mathematical modeling and simulation of SOFCs is a time-consuming process (even with today's computers), involving some

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level of uncertainty. Usually some physical, chemical and electrochemical properties and detailed structural properties are unknown, requiring some assumptions or estimations to solve the mathematical model. On the other hand, ANN models are much faster when trained by experimental data and therefore do not require access to the unknown parameters. ANN models have to be trained properly and after that they will predict the response of the SOFC quickly. This fast response of ANN models makes them ideal for use in SOFC control and monitoring tools.

Few attempts have been made to show the ANN data-driven models' strengths in SOFC modeling and control. In most of these works the proposed ANN model has been trained using simulation data, which are usually limited, compared to experimental data that can have thousands of training samples. Arriagada et al. [22] trained a two-layer feed-forward ANN with a data set from a mathematical model. Then they predicted air flow, current density, mean solid temperature and outlet temperatures. Jemei et al. [23] presented an ANN model for a proton exchange membrane fuel cell (PEMFC). They had an experimental set-up and used measured data for the training and validation of their model. In another work on the ANN modeling of a SOFC, Milewski et al. [24] used published experimental results to train a two-layer network with nine inputs, seven neurons in the hidden layer and one output. They merged measurements from at least two different set-ups with different structures and materials to train their model. Consequently, there are serious doubts about the consistency of their training data. The idea of a neural network hybrid model was presented by Chaichana et al. [25]. They combined the mass conservation equation with a neural network and predicted the distribution of gaseous species in the fuel and air channels. They used simulation data for training their network. Radial basis function (RBF) neural networks are also used for SOFC modeling. Wu et al. [26,27] developed an RBF neural network based on genetic algorithm (GA) and trained it using simulation data from publications. They showed the possibility of using their model in a predictive control program [28]. Genetic programming (a specialization of GA) is also used for SOFC modeling using a simple mathematical model for generating the training data [29]. The performance of an ANN and Adaptive Neuro-Fuzzy Interference System (ANFIS) for modeling a tubular SOFC stack was studied in Entchev et al.'s [30] work. Experimental data from a 5 kW micro-generation SOFC system was used in their study. The maximum relative error of both methods was about 10%, but the ANN model was faster than the ANFIS.

In this study a multilayer feed-forward neural network with error back-propagation was chosen for modeling a stack of a six-cell planar SOFC. A test rig was set up for generating the training data for the ANN model. Five temperature sensors were mounted inside the cell for local temperature measurements. Current and voltage data were also measured and recorded simultaneously. Air flow, fuel flow, fuel composition, oven temperature and current were varied during the test (in a specified range) in order to gain more complete knowledge of the stack's behavior. The temperature profile of the middle cell and the cell voltage were recorded as the outputs of the system. ANN models with different numbers of neurons in the hidden layer were tested to select the optimum structure of the network.

2. Experimental set-up

An experimental set-up was built, consisting of a cross-flow type stack of six cells. Fig. 1 shows the assembled stack. Table 1 shows the geometrical specifications of the cells. The MEAs (membrane electrode assemblies) were 3YSZ electrolyte supported cells from Kerafol, Ni/YSZ nickel cermet anode and LSM cathode. The ceramic interconnect was made of doped lanthanum chromite

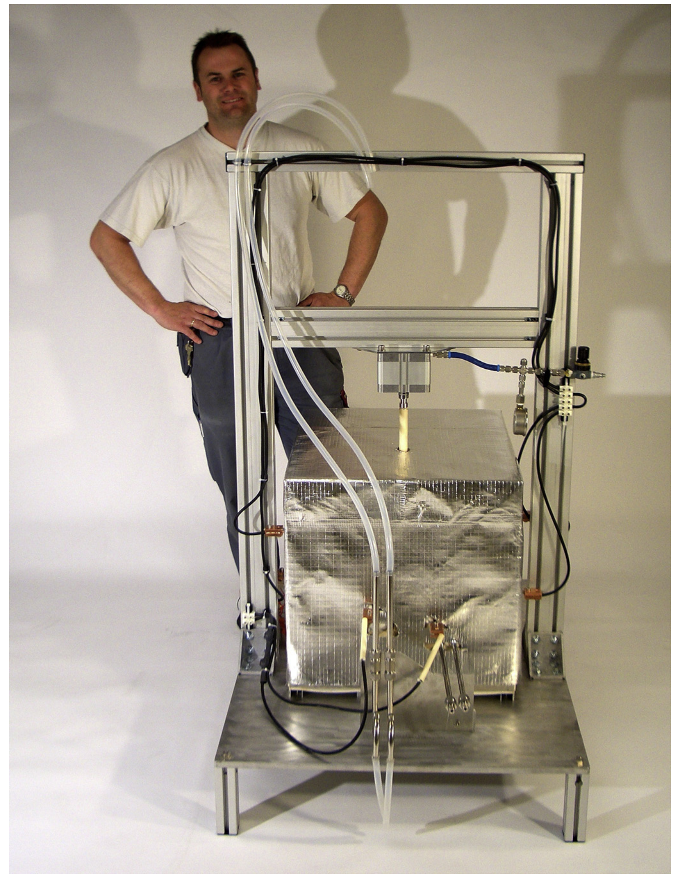

Fig. 1. Test rig.

($LaCrO_3$). Five thermocouples (type K, ϕ 0.5 mm) were inserted inside the middle cell to measure the temperature at the four corners and in the middle point of the cell. Fig. 2 shows the temperature sensor configuration and sensor labels. The stack was put in the oven, which had a temperature control system. For the current densities between zero and 0.1 A cm^{-2}, the cell voltage and five temperatures were recorded. Air and fuel were supplied at atmospheric pressure. The details of this experimental set-up and test results can be found in our earlier work [31].

3. Test procedure

The goal of this test set-up was to investigate the effect of current and oven temperature on solid oxide fuel cell performance. By changing the oven temperature and electrical current, different test points were defined. During the test program, the following data

Table 1
Fuel cell geometry.

Geometrical parameters	
Cell width	86 mm
Cell length	110 mm
Channel width, fuel and air side	3 mm
Channel height, fuel side	0.40 mm
Channel height, air side	1.20 mm
Anode thickness	50 μm
Cathode thickness	70 μm
Electrolyte thickness	150 μm
Number of air channels	22
Number of fuel channels	27

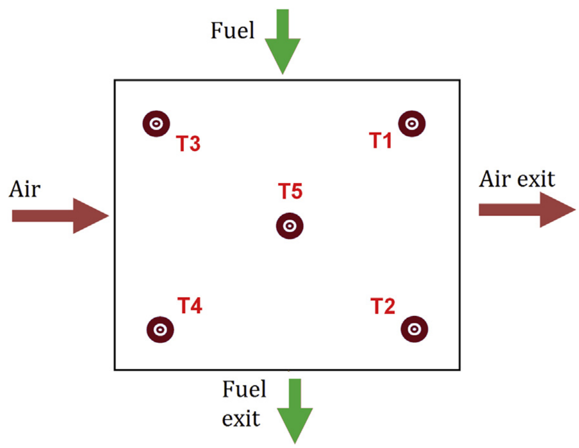

Fig. 2. Temperature sensor position.

were recorded: five temperatures from the middle cell (Fig. 2), one oven temperature and five voltages (anode current collector voltage, cell no. 2 voltage, cell no. 4 voltage, cell no. 6 voltage and cathode current collector voltage). In Table 2, the setting parameters are shown. A large amount of excess air was used to limit thermal gradients in the stack [32]. Fuel utilization was kept low to prevent high current densities and thus avoid degradation.

The preparation of the stack for the test is a very sensitive procedure. Any change in the operating conditions of the cell should be made slowly to avoid unnecessary shocks to the sensitive structure of the solid oxide fuel cell. A mixture of hydrogen, nitrogen and carbon dioxide was used as fuel for the start-up in the open circuit condition. The furnace temperature was increased gradually at the rate of 25° per hour. When the temperature reached the defined value and became stable, H_2 flow increased from 500 to 1000 ml min^{-1} gradually (in more than half an hour). After these steps and a period of stabilization, the current was changed step by step from zero (open circuit) to 10 A. All the measured data were recorded every second during the whole process, and the overall test history was logged.

For starting the test and obtaining the required data, nitrogen flow was gradually omitted from the fuel, and hydrogen was increased to reach the desired flow rate. The test was started with an oven temperature of 900 °C, and current was changed from zero to 10 A. This procedure was repeated for 900 °C and 1000 °C oven temperature.

4. System description

Temperatures (five temperature measurement points) and cell voltage can be considered as the output of the system because they are responses of the system to the input settings. The input settings are the amount of air and fuel we put into the cell, the oven temperature and the electrical current. Fig. 3 shows our system in a block diagram with its inputs and outputs.

Table 2
Test set-up parameters and their variation ranges.

Setting parameter	Range of variation
Air flow (l min^{-1})	45.0
H_2 flow (ml min^{-1})	500–1000
N_2 flow (ml min^{-1})	0
CO_2 flow (ml min^{-1})	1000
Oven temp. (°C)	900–1000
Current (A)	0.0–10.0

Fig. 3. SOFC block diagram.

In this block diagram, fuel input is simplified and shown as "Fuel". However, as our fuel was in fact a mixture of three different gases (H_2, N_2 and CO_2), in our model it is divided into two different inputs: one for H_2 and one for N_2. The CO_2 is ignored in this model because it was not changed during the test. Air is also a mixture of oxygen, nitrogen and other gases but, since that composition was not altered, it was simply presented by one input parameter. Therefore, this model consists of five inputs and six outputs.

The outputs of the system are good indicators for use in a monitoring system. Cell voltage predicts the performance of the system. On the other hand, the temperature estimation for five different points in the cell gives an approximate temperature distribution which then can be used as the indicator for healthy operation of the stack.

5. Data processing

Since the events in this test took place in a slow rate, the training data was averaged every 30 s. Fig. 4 shows different measured outputs of the system. Observing this figure, some outliers in cell voltage data can be seen. Also, around time step 1250, there are several points out of the normal range. To find the reason for this behavior, the history of the data was reviewed. The area ranging from 750 to 1250 is the response of the system to the oven temperature increase from 900 °C to 1000 °C at constant rate. At the end of this period, one of the voltage measurement electrodes recorded some tenth of volts less than the expected normal range, which caused a larger voltage difference between two cells. Since this was recorded just for one of the sensors, it was concluded that this was not a normal response of the system. This could be caused by loss of contact between the voltage measurement sensor and the fuel cell current collector as a result of the changing temperature. Therefore these outliers were filtered out before ANN modeling.

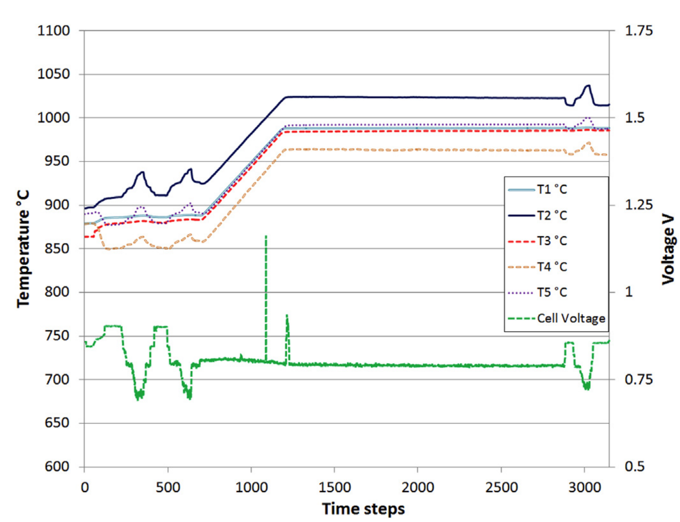

Fig. 4. Measured output of the system (30 s averaged).

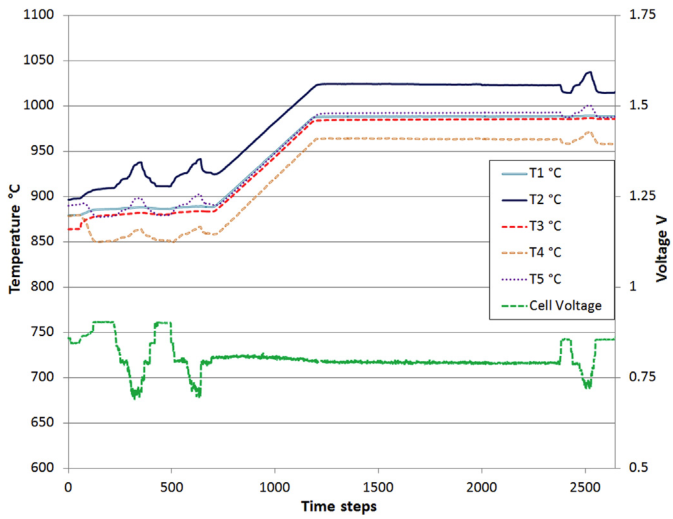

Fig. 5. Filtered data for training.

Table 3
Randomization check.

	Training	Cross-validation	Test
Maximum temp. (°C)	984.096	984.093	984.07
Minimum temp. (°C)	867.736	867.699	867.826
Maximum current (A)	10.0124	10.0108	10.0114
Minimum current (A)	−0.003014	−0.003013	−0.002972

Time steps 1800–2800 (Fig. 4) represent the night time, with the stack operating at constant conditions. If data for the whole of this period was included in the training data, then the ANN model response tended to be closer to this condition, which was not desirable. Therefore the data between time steps 2000 and 2500 was left out for better model generalization capability.

The filtered data set, containing 2625 rows of data, was obtained and used for training the ANN model. The filtered data is illustrated in Fig. 5.

Apart from this set of data, used for training, other data sets were taken out for evaluation and control of the accuracy of the ANN model. These evaluation sets were not introduced to the model during the training procedure. The evaluation data sets were selected in such a way that permitted a check of the extrapolation capabilities of the model containing measured data collected at the beginning of the test. Hydrogen flow was 300 ml min^{-1}, air flow was around 14 l min^{-1} (one third of the normal air flow) and a

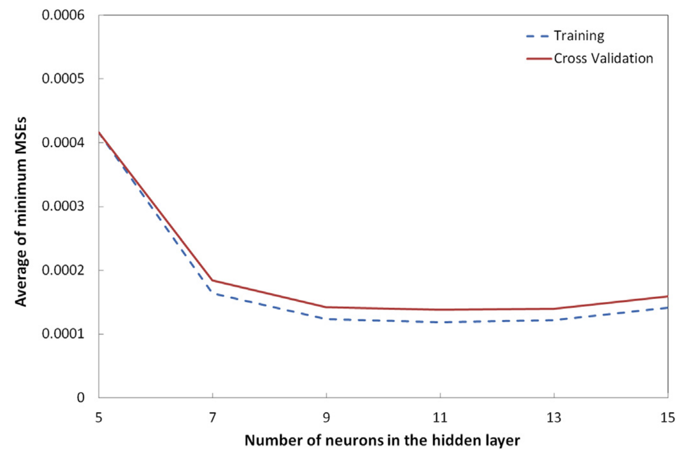

Fig. 7. Variation of number of neurons in the hidden layer.

considerable amount of nitrogen (500 ml min^{-1}) was fed to the fuel stream. There was zero current across the cells (open circuit).

6. Modeling

NeuroSolutions for Excel™ module (version number 5.07) was used to create and train the artificial neural network. This module is a great tool for small to medium-size neural networks. Microsoft Excel™ has a limit of 65,000 rows, but the data set used in this study comprised less than 3000 rows of data and thus that limitation did not cause any problem.

To obtain a good generalization, it is highly recommended to randomize the data rows in order to gain a more complete representation of data in each subset [21]. After the randomization, the presence of both maximum and minimum values of air temperature and current (the two most important input parameters) in all three subsets were checked; see Table 3. In this model, rows of data were randomized using NeuroSolutions module in Excel™. The data set was divided into three subsets: training, cross-validation and testing containing 60%, 15% and 25% of the whole data, respectively [21]. Each subset has a certain effect on the training procedure of the network. The training subset is used to generate errors during the training process and hence update the weights. The cross-validation subset ensures that the network does not become over-trained. The training is stopped when the mean square error (MSE) in the cross-validation set starts to increase. The test subset, which is not used during the training, is employed after the training to examine the generalization capabilities of the

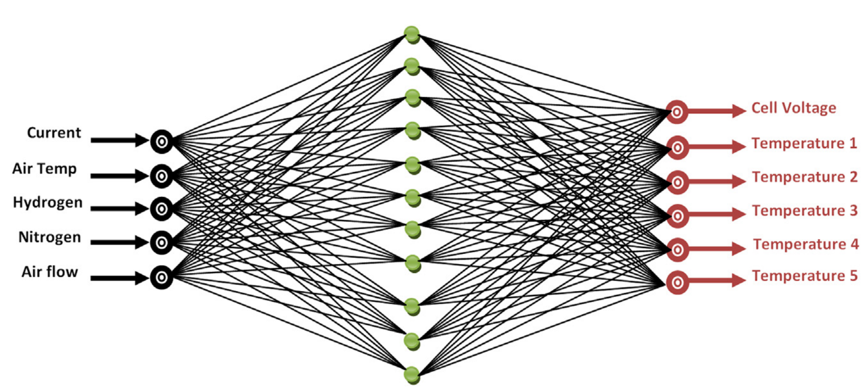

Fig. 6. Optimized neural network structure.

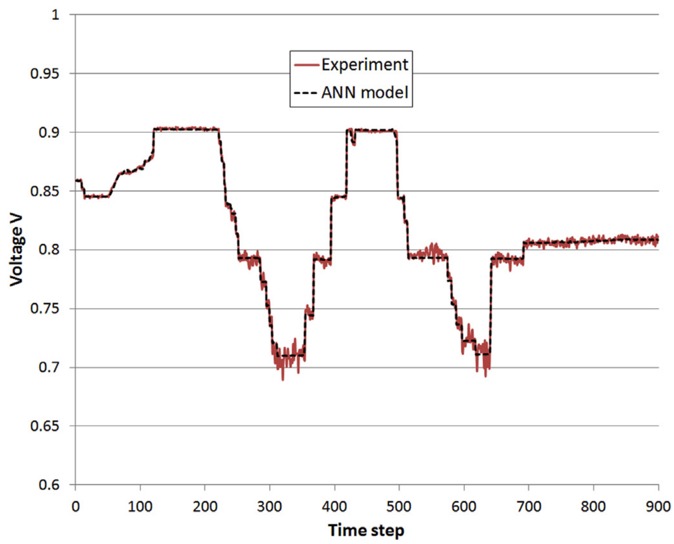

Fig. 8. Cell voltage comparison between ANN model and experiments.

network and to compare with the other errors (training error and cross-validation error). All three errors should be similar [19].

The ANN used in this study is a fully connected one hidden-layer feed-forward network with back-propagation learning algorithm. The supervised learning control was activated for early stopping of the training procedure, before the network becomes over-trained. The tangent hyperbolic transfer function was selected for axons. Improved gradient descent learning method (back-propagation) was used to find the synaptic weight values. This method has been shown to perform well in regression problems [19,20].

The number of neurons in the hidden layer was optimized during the training process. Due to the number of inputs (5) and outputs (6) the number of neurons in the hidden layer was varied between 5 and 15, and the best network structure was selected. This range of neurons proved to be sufficient for the optimal solution.

Quite a high number of epochs was chosen (over 15,000). An epoch is defined as one complete presentation of all the data. This number ensures reaching a good regression (with acceptable error) and, in combination with the early stopping method, means that the training time will not increase dramatically.

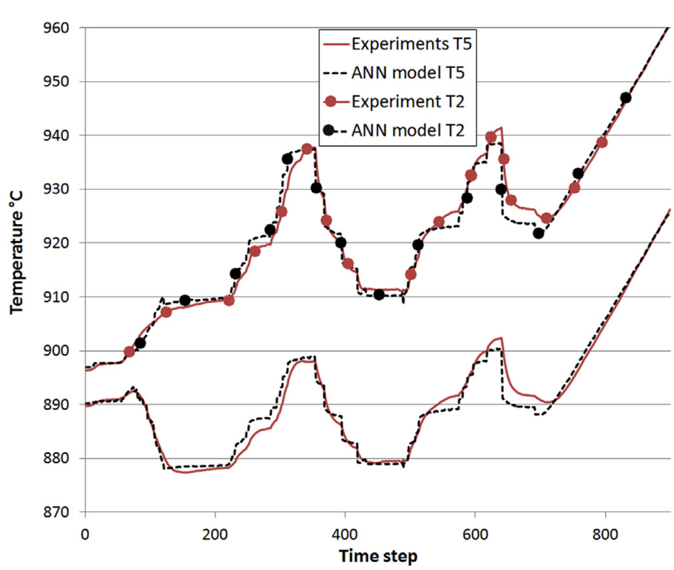

Fig. 9. T2 and T5 temperature comparison between ANN model and experiments.

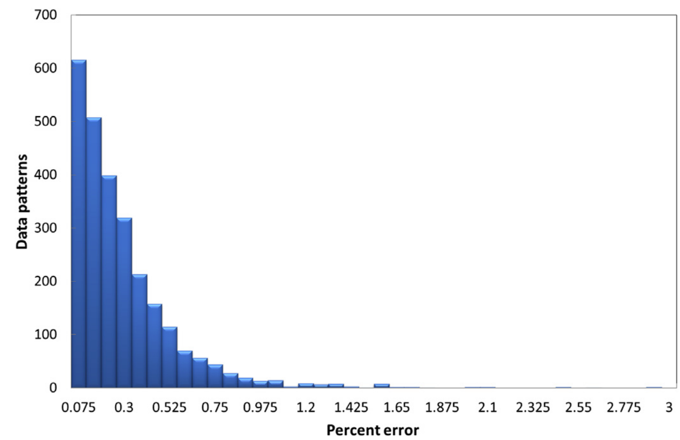

Fig. 10. Distribution of the error of the voltage.

This explained training procedure was repeated for the same randomization but with small changes in the initiated weight values to minimize the probability of converging to local minima. Although the randomization performance was checked and showed a good representation of data, a second randomization was also performed. Two other training processes were performed based on this new randomized set of data. Finally, the best network among all the obtained networks was selected.

7. Results and discussion

The training process was carried out with a variation of 5–15 neurons in the hidden layer and 20,000 epochs. The optimized structure for the ANN model was found as: 5–11–6. This refers to 5 inputs, 11 neurons in the hidden layer and 6 neurons in the output layer. Fig. 6 shows a graphical representation of this network. Training with more than 11 neurons in the hidden layer resulted in the increase of the cross-validation and training errors. This can be seen clearly in Fig. 7.

Figs. 8 and 9 show the ANN prediction of the stack outputs (voltage and temperatures) against the measured data. Since the performance of temperature prediction is very similar for all five temperatures, only T2 and T5 prediction performances are shown in Fig. 9. As can be seen in these graphs, the ANN model successfully predicted the dynamic response of the system. The average relative error was only 0.2% for voltage prediction and 0.05% for temperature prediction. The maximum relative error was 2.6% for cell voltage and 0.7% for temperature. The maximum relative error for

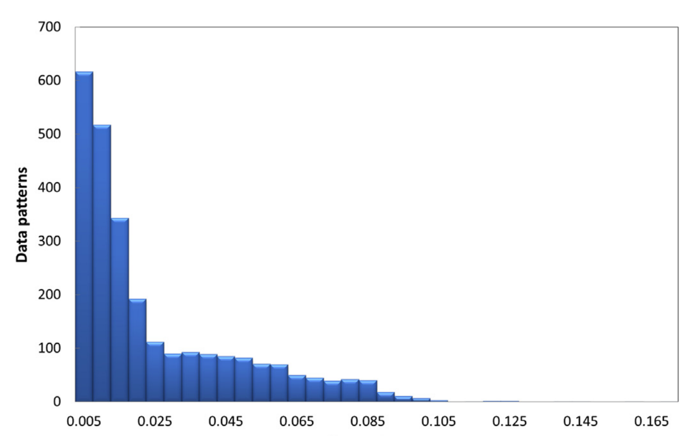

Fig. 11. Distribution of the error of the T1 temperature.

Table 4
Input parameters for generating extrapolation data.

Setting parameter	Range of variation
Air flow (l min^{-1})	15.0
H_2 flow (ml min^{-1})	332
N_2 flow (ml min^{-1})	500
CO_2 flow (ml min^{-1})	1000
Oven temp. (°C)	867
Current (A)	0.0

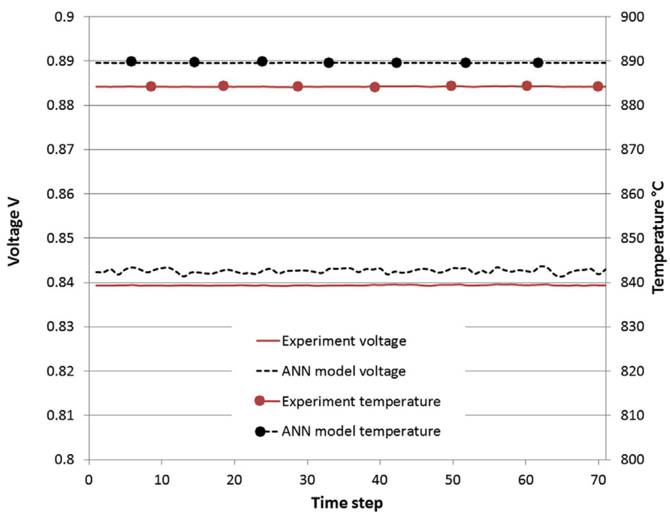

Fig. 12. Voltage and temperature comparison between ANN model and measurements for a data set out of the training range.

temperature prediction was better (around 1%) because of the less noisy measurement data. The error distribution for voltage and T1 temperature is presented in Figs. 10 and 11, respectively. The figures show the quality of the ANN prediction. For example, in Fig. 10 it can be seen that the error is above 1% for only a few data patterns.

The response of the ANN model to a data set completely out of the training range was also studied. A data set from the beginning of the test was used for checking the extrapolation capabilities of the ANN model. Input parameter values are shown in Table 4. Temperature and voltage predictions are compared to the measurements in Fig. 12. It can be seen that the accuracy of the prediction is reduced, but the model is still able to give comparable results to the measurements.

8. Conclusion

The ANN modeling approach was successfully demonstrated for a short SOFC stack. The prediction of the voltage and local temperatures was more accurate than in the case of complicated computational fluid dynamics (CFD) models (for example, please refer to our previous work [33]). This high quality of prediction, along with the very fast response of the model, makes the ANN model a serious competitor for use in the heart of a stack control and monitoring tool. Models for model based control application should be very simple and fast and at the same time they should have good accuracy, all of these conditions are not usually met for mathematical models.

The combination of the local temperatures and voltage predictions provides a good indicator of the working conditions of the stack. Monitoring tools can use this information to advise operators whether the stack is working normally or is going to fail. The proper action can be taken for safe operation of the stack, manually or automatically.

Neural networks are not usually so strong in extrapolations. However, in this study the ANN results for an unfamiliar set of data is still in good agreement with the measurements. Introducing more training data for a wider range of operation will increase the prediction accuracy of the model considerably.

ANN models also have some limitations. They are tailor-made for a specific set-up and therefore not applicable to a different system without being trained with the new system's data. However, it is possible to train an ANN model for a prototype SOFC stack and then apply it to the commercial stacks with good reliability. Moreover, a large amount of experimental data is usually required for training the ANN. Simulation data generated by mathematical models can also be used for covering more operational points for training the model, but some experiments for validating the simulation results are necessary.

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